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Validation of Complex Rate-Dependent Material Constitutive Models

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Abstract

Constitutive models for rate-dependent materials can be little more than a curve fit of the experimental stress-strain behavior, or they can be complex models based on a micro-mechanics analysis of the micro-mechanisms believed to be physics controlling the rate dependence. In all cases, they are based on observational data for tests conducted at different loading rates, temperatures, and stress states. The strain rates that various parts of the geometry experience can range over several orders of magnitude for models that are used for even relatively simple geometries and loading conditions. If the structural response modeling is to be accurate, the constitutive model must also be accurate over several orders of magnitude of strain rate. The constitutive model for a polymer-based explosive, PBX 9501, used in surety and safety studies has been reported in [1,2], and is known as ViscoSCRAM. This model is a rate-dependent Finite Element (FE) material model made up of generalized parallel Maxwell elements to represent the rate-dependence which are combined with a rate-dependent damage law that is based on statistical crack growth mechanics per unit volume of material. Validation for such models is very important if they are to be used with confidence. In this paper, we show that modeling the Split-Hopkinson Pressure Bar (SHPB) test using the newly emerging technology available in massively parallel FE computations can be used to validate them [6]. As the technology-transfer from the Department of Energy (DOE) via the National Laboratories to Industry that is coming out of the Advanced Strategic Computing Initiative (ASCI) program becomes available, large-scale calculations will become commonplace. In this paper, a methodology is presented that demonstrates the promise of this technology that can be a "template" for validation of complex rate-dependent material models.

Introduction

The ViscoSCRAM Constitutive Model for the mechanical behavior of high explosives has been developed for both explicit FE technology [1] and implicit FE technology [2]. ViscoSCRAM also has been used as a FE constitutive model to represent other rate-dependent materials (i.e. other than high explosives) that exhibit visco-elasticity and rate-dependent damage effects. As an aside, a parallel paper is in preparation on how to determine the parameters for this model (number and type of experimental tests required, as well as how to analyze the experimental data to arrive at the ViscoSCRAM parameters for a given material). We will use the ViscoSCRAM model in this paper to illustrate how to validate a complex rate-dependent material model. In current day ASCI nomenclature, a "model" must be both "verified" (the programming represents the theory correctly) and "validated" (the theory represents the physics correctly) before being released with confidence to the "user" community for modeling complex phenomena in massively parallel ASCI computer programs. Currently, massively parallel computational capability is available at the three National Laboratories, Los Alamos, Sandia, and Livermore, and at some selected universities. However, as the technology becomes more commonplace, the analyst will be able to simulate the very complex structural behavior experimentally observed. It can also be expected that the material models available for these simulations will be ever more complex, and will include much more micro-mechanical behavior, and if the models are validated, the analyst can begin to believe the results of the simulation with some confidence. Currently, there is an AIAA standard in existence on computer code validation for fluid dynamics, and an ASME committee that will address yet a different standard for validation of computer codes used for solid mechanics [3,4]. These standards will undoubtedly help the "user" community by assuring that the codes they select can be used with confidence in their predictions. However, the material model developer must also be concerned about validation of the model that is developed if it is to be released to the user community as a "production code" model rather than a research tool.

The ViscoSCRAM Material Model

The theoretical development of this model and some applications for it have been put forth in the previous publications cited as Ref. [1,2] and the reader interested in the theoretical development is referred to those publications for the full details. The schematic representation of the model is given in Fig. 1, which illustrates that the deviatoric strain is decomposed into a visco-elastic contribution and a statistical crack size growth contribution. The law governing the rate at which the average crack size per unit volume grows is a function of the effective strain rate in the current versions of ViscoSCRAM.

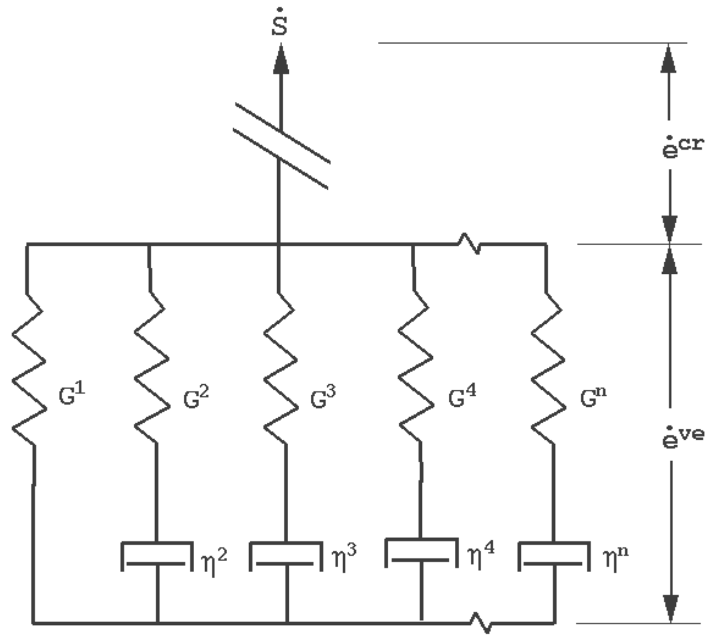

Figure 1 Schematic representation of the ViscoSCRAM material model for rate-dependent materials that experience rate-dependent damage. The total strain rate is composed of a visco-elastic contribution and a cracking damage contribution.

Current versions also include tensile average crack growth with a different damage growth rate law in tension than compression. The material model is available in several "production" versions of the FE programs used at Los Alamos to model structural response and safety studies for systems involving high explosives. These production codes include the widely used explicit programs DYNA3D, PRONTO3D, and ABAQUS Explicit, and the implicit versions, ABAQUS Standard, and some local implicit versions. The model has had extensive validation against available experimental data for the material known as PBX 9501, and some of these studies have been illustrated in [1,2]. However, the model parameters have also been determined for other materials. For example, a composite comprised of barium nitrate with a nitroplasticized-estane binder material called Mock 900-21 is used as a mechanical mock material for PBX 9501 in some types of safety-related experiments. The mechanical properties have been determined for this material from uni-axial stress-strain experiments, using quasi-static strain rate and high strain rate Hopkinson bar experiments in compression. Using the ViscoSCRAM material model with the parameters determined from analyzing the test data, the uni-axial experiments were simulated using a FE code. Fig. 2 illustrates the comparison between the low-rate tests at room temperature and the model and shows a higher rate curve from the model for a Hopkinson bar rate (1400 /s).

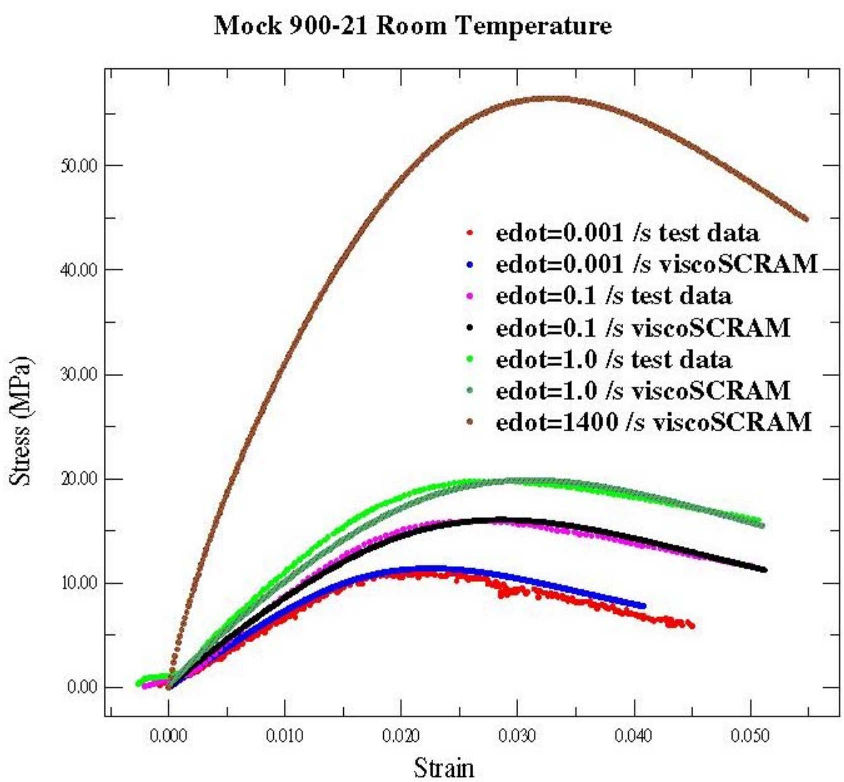

Fig. 2 Uniaxial stress strain result from ViscoSCRAM compared with experimental low-rate test data for Mock 900-21.

The Hopkinson-bar tests do not automatically produce a either uniform uniaxial stress state of stress or a constant rate stress-strain curve. Such a curve must be deduced from a number of tests and data analyses with different Hopkinson-bar sample aspect ratios and impact velocities. An example of the raw data from a Hopkinson-bar test for this material is shown in Fig 3.

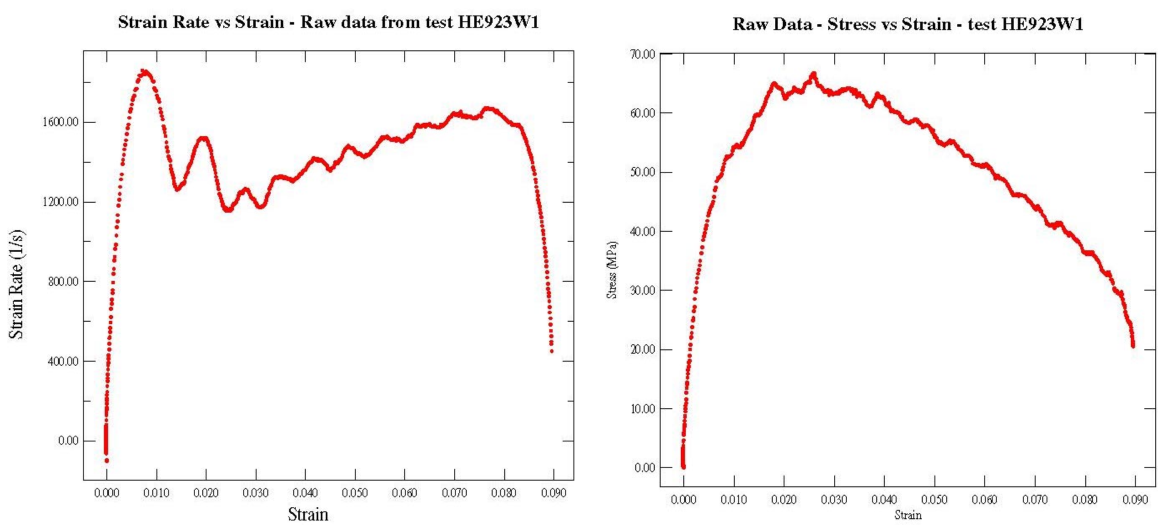

Figure 3 Plots of raw data from a room temperature compressive Hopkinson-bar test of Mock 900-21.

The left-hand plot shows the strain-rate vs. strain records and the right-hand plot shows the stress vs. strain from the data for a given test that reached stress-state stability in the specimen at a rate of about 1400 /s. Part of the objective of this paper is to illustrate another methodology for using Hopkinson-bar data in FE simulations.

ViscoSCRAM for PBX 9501

The ViscoSCRAM model with the mechanical parameters determined for the polymer-based explosive, PBX 9501, has been used to model available mechanical-property constitutive experiments for model verification purposes. Parameter studies have also been carried out to illustrate the effect of varying from the recommended ones for this material. Features of the model and the results of some of these studies will be illustrated using PBX 9501 parameters for illustration.

Figure 4 shows the simulation results of ViscoSCRAM using recommended parameters for constant rate compression tests with rates in the range achievable with a standard mechanical testing machine. The nature of the rate dependence of this material is clearly exhibited in this figure.

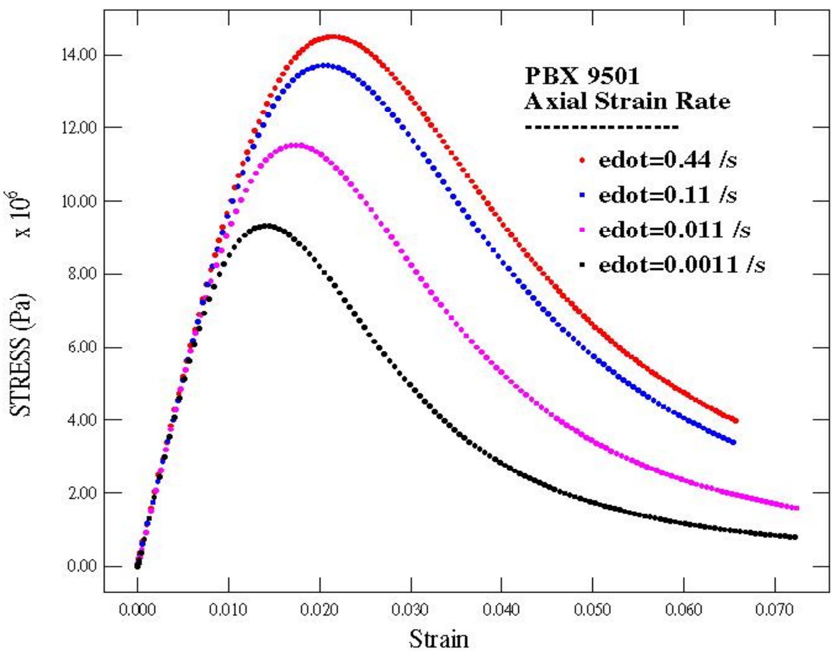

Figure 4. ViscoSCRAM predictions from simulating the uni-axial stress-strain tests reported by Idar, et.al. in Ref . 6.

The damage law used in ViscoSCRAM requires the instantaneous average crack growth rate to be a function of the effective deviatoric strain rate, a scalar measure defined as a constant multiplying the square root of the inner product of the deviatoric strain-rate tensor with itself. The form of the damage law is given in Eq. (1).

$$\log(KV_{\max}) = \log(\dot{e}deff) \tag{1}$$

The damage law that is recommended for PBX 9501 is shown in Fig. 5 and the points on this figure that *correspond to the test data* that was used to determine the law are also shown. The multiplier K in Eq. 1 depends upon whether the stress state is in tension or compression and $V_{\max}$ is a relatively complicated variable that depends upon the value of the stress intensity factor in the statistical crack analysis development. The reader interested in the details is referred to Equations 24-31 of [2].

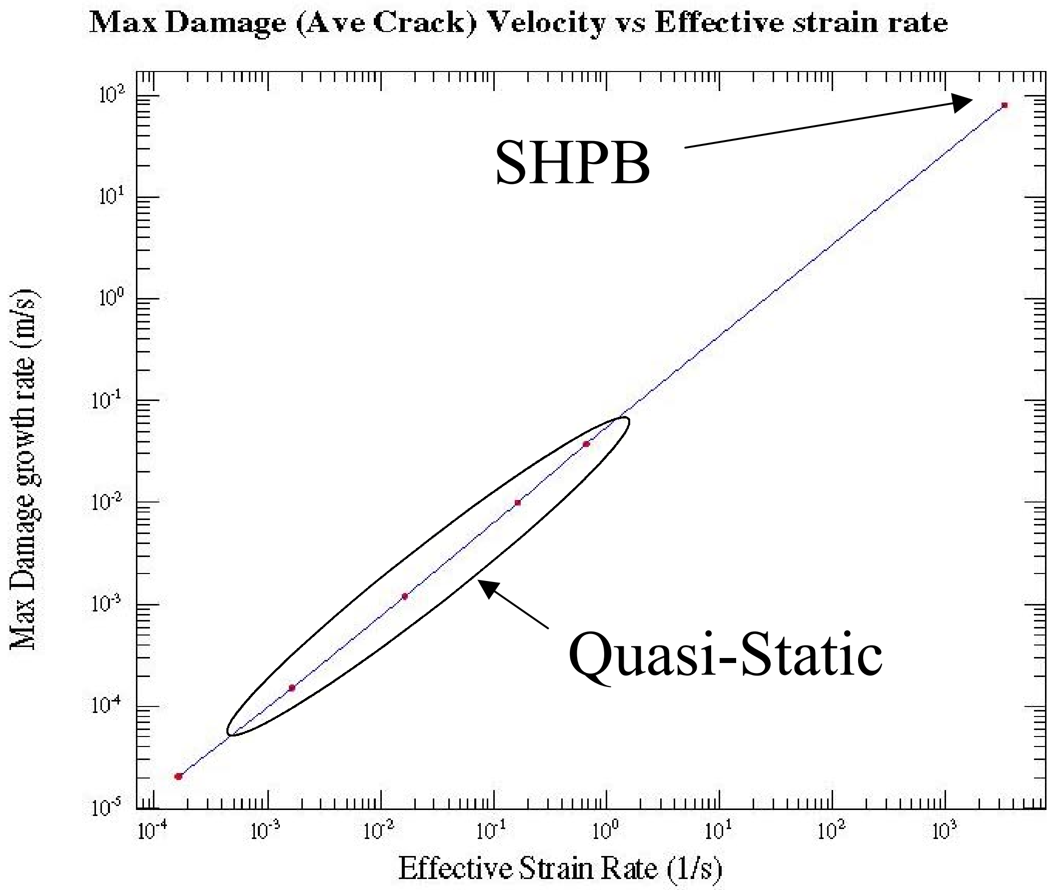

Figure 5. The damage law recommended for PBX 9501.

There are two physical interpretations to the damage law in the ViscoSCRAM material model. One interpretation is that the local value of the damage variable is the predicted total amount of average crack growth per unit volume that has occurred over the total number of average sized micro-cracks that the material has per unit volume initially. For example, an analysis may predict that the damage variable has a size of 10 mm. This value would indicate that N micro-cracks that began with a characteristic average radius of 1 mm have grown to 10 mm average radius. This value should not be interpreted to mean that a single micro-crack is now 10 mm long, but rather that the total average crack growth is that value, so that the average crack growth per unit volume is 10/N in size. Another way of saying this is that *the effect of the damage from micro-crack extension* is 10 times the effect that the initial micro-crack field has on the material's mechanical properties.

There is yet another physical interpretation of the average crack radius as a damage variable. This interpretation is indicated in Fig. 6. Figure 6 shows the axial stress from all of the uni-axial stress-strain tests plotted vs. the normalized damage parameter, c/a . The relationship between c and a is given in Ref. 2, but basically, a is an average initial flaw size and c is the current flaw size for N_0 flaws per unit volume. This second interpretation is in terms of the remaining "strength of the material" when the normalized damage parameter exceeds unity as illustrated in Fig 6.

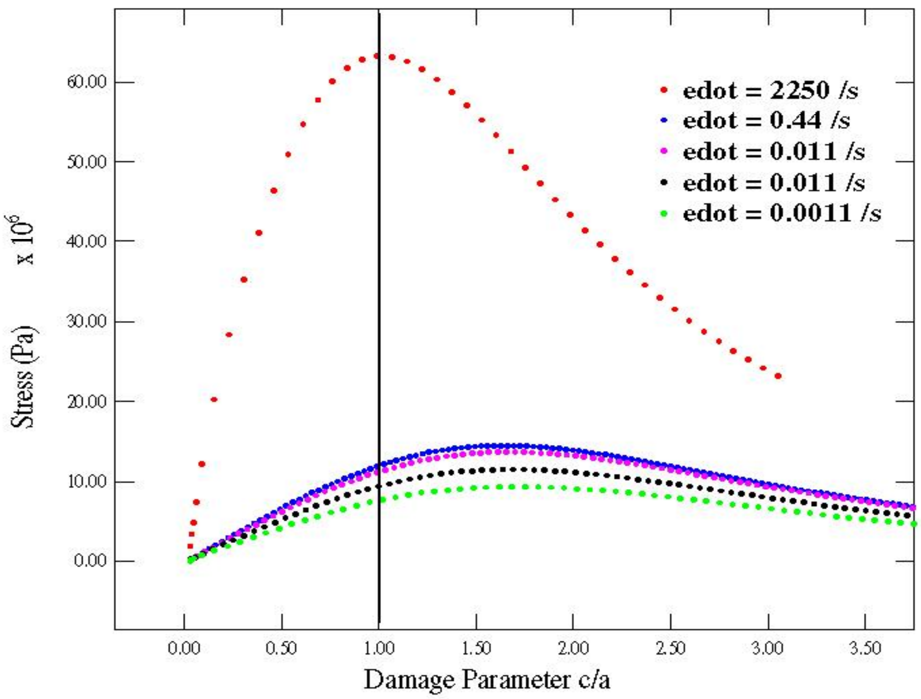

Figure 6. The "remaining strength" interpretation of the damage parameter. The "strength" tends to peak at a value of one at higher rates and "is peaking" at a value greater than one for lower rates.

Some of the features of ViscoSCRAM have been exhibited above, and the sensitivity of varying the input parameters is given in the FE program manuals that are available for each implementation. The reader interested in this material is referred to those documents. The purpose of the illustrations above is to show that the material model is indeed a complex material model featuring rate-dependent response and rate-dependent damage and should be validated extensively against experimental data.

Validation of ViscoSCRAM – A Methodology for Complex Rate-Dependent Models

The parameters for *all* material models are ultimately determined from experimental data. Rate-dependent materials are *recognized* from well-instrumented experiments carried out at varying strain rates and temperatures. As already stated, even in simple geometry applications involving structural dynamic or quasi-static loading FE simulations, the strain rates in the geometry at a given instant will vary over orders of magnitude.

For validation, a rate-dependent material model should be implemented in both implicit FE programs and in explicit FE programs. Low-rate test data from experiments that follow standards for specimen geometry, specimen end lubrication recommendations if in compression, and good instrumentation and data reduction practices, can be most accurately simulated using an *implicit* program. These programs require that the incremental tangent stiffness is formed, and one method of forming it for complex rate-dependent models is given in detail in [2].

Validation at Low Rates

The lower rates of test data available for determining the parameters for these models will generally range from 0.001 to 1 per second for a testing machine that has good rate control. Rates lower than this range, tend to be creep tests and these tests are generally done under load-control rather than displacement-control.

Once the FE model parameters have been determined, then the compression tests should be modeled using velocity or displacement boundary conditions that will give the correct strain rate. The material model stress-strain response is then exhibited against the experimental test data such as has been done in Fig. 2 for Mock 900-21. Other examples of such validation of ViscoSCRAM for PBX 9501 were shown in [2]. In that reference, it is demonstrated that by having an *implicit* model implementation, the simulation of low rate experiments that have complex stress states is possible. Another example is shown in Fig. (7) of the ViscoSCRAM modeling of a modified formulation of PBX 9501 using the result from an implicit code. The excellent correspondence between the FE simulation and the actual experimental curve is strong validation of the model at low strain rate.

Validation at Higher Rates

Validation of the material model at Hopkinson-bar strain rates is not so easily done because often the experiment does not achieve a *constant strain rate* as shown in Fig. 3 for materials that undergo damage processes. Therefore FE simulations of the Hopkinson-bar must account for this variable strain rate behavior. In addition, the specimen initially must reach stress-state stability for the data to be valid by ringing up so that the magnitude of the stress at both specimen interfaces should be approximately constant. This equilibrium condition is verified for a given test by agreement between the 1-wave and 2-wave analysis. As explained in [5], the 1-wave stress analysis uses only the strain gage data from the transmitted bar to calculate the stress and represents the specimen stress at the interface with the transmitted bar. The 2-wave stress is obtained from an analysis of the incident and reflected wave forms and represents the specimen stress at the interface with the incident bar. If these two analyses do not agree, then a uniform (uni-axial) stress state is not achieved throughout the specimen and the experimental data is invalid until agreement is achieved.

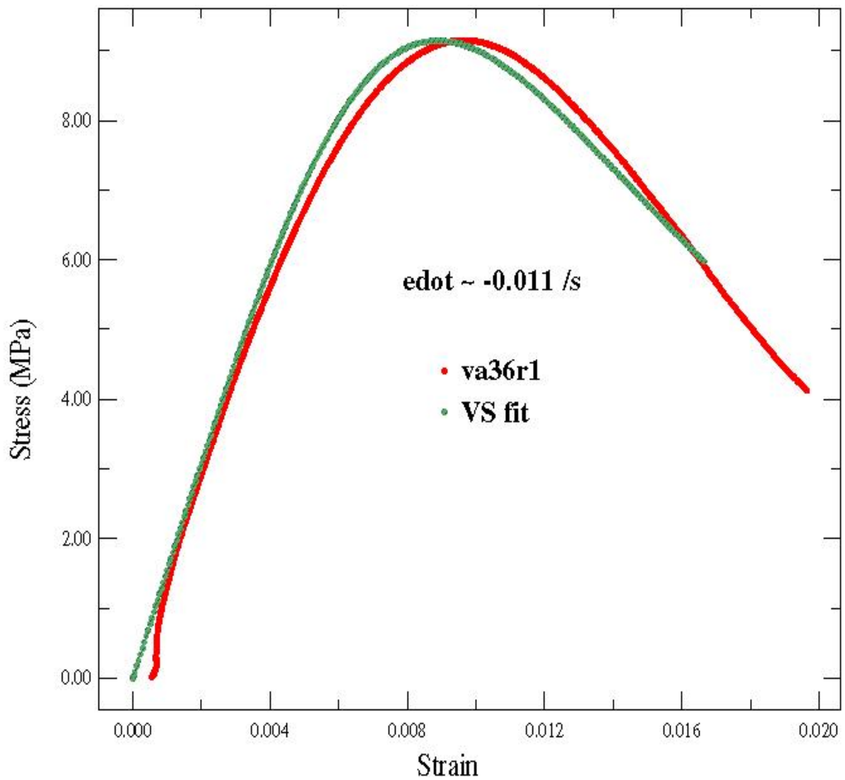

Figure 7. A simulation of a low rate test for PBX 9501 using the model parameters determined for this particular formulation of the material. The "fit" *is the simulation* and is part of the validation procedure.

The basic compression Hopkinson-bar configuration used at Los Alamos is shown in Fig. 8. Different bar materials are used with hard and soft test material samples, the choice being dependent upon the magnitude and duration of the desired stress, strain and strain rate states in the sample. For PBX 9501, the bars utilized were a titanium alloy, Ti-6Al-4V,[6,7]. The properties of these bars are given in Table 1.

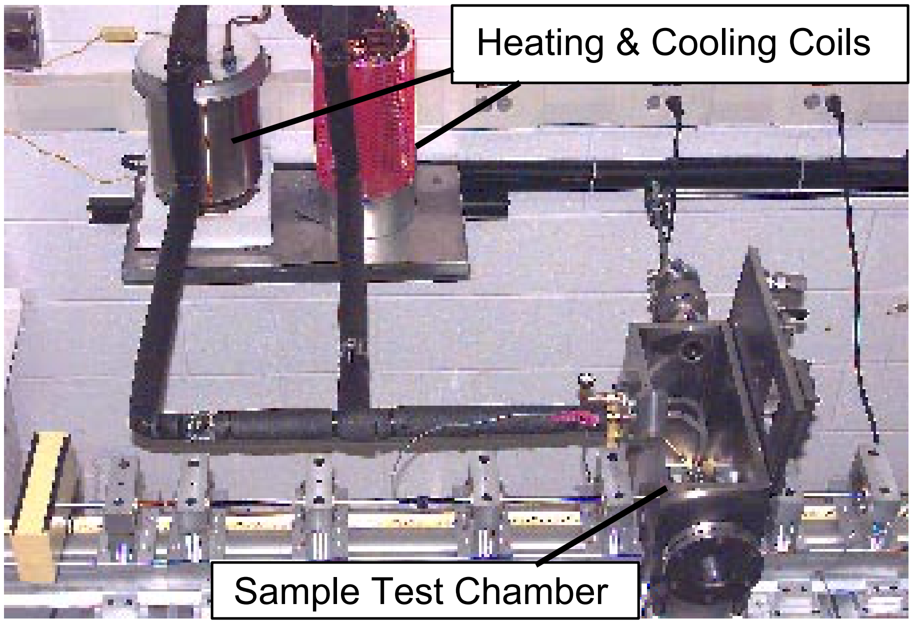

Fig. 8 LANL – Split-Hopkinson Bar Facility specially designed to test energetic and polymeric materials, Ref. (6).

Table 1 Typical Hopkinson-bar Properties for PBX 9501 Experiments

Striker Bar Length	150.25 mm
Incident Wave and Transmitted Bar Lengths	760 mm
All Bar Diameters	9.470 mm
Bar Rod Sound Speed	4867 m/s
Density	4.429 g/cc
Poisson Ratio	0.34
Strain Gage Locations	Mid-bar for both
Bar Young's Modulus of Elasticity	105 GPa

Just as for the low-rate validation modeling illustrated above, the high-rate experiments should be modeled to validate the material model. Without the newly emerging massively parallel computational technology, full 3-dimensional modeling of such an experiment has been impractical if not impossible in the past. However, if the model is implemented into a 3-D simulation code, then the validation should be carried out in that space and such validation will be illustrated here.

The finite element model mesh configuration of the test geometry is not shown here because the length scale compared to the bar diameters is so large that it appears only as a line, graphically. However, a "zoom-in" on the PBX-9501 specimen as modeled is shown in Fig. 9. In the validation simulation that will be described, this material is modeled with the ViscoSCRAM material model.

The strain gages in this model are simulated at the midpoint of the incident-wave and transmitted-wave bars using thin shell or membrane elements that share the same nodes as the continuum elements that make up the outer surface at these locations. Their properties (modulus, thickness, etc) are set such that they contribute no stiffness to the elements to which they are "bonded". These elements simply follow the titanium bar motion, just as strain gages do.

The simulations illustrated in this paper uses ASCI Technology and the LLNL explicit FE program called PARADYN, a massively parallel version of DYNA3D, [8]. The FE model contains about 2.1 million hexagonal 8-node brick continuum elements with about 65,000 elements in the PBX 9501 sample. The bar is modeled in quarter symmetry, with appropriate symmetry boundary conditions on the symmetry faces. All material interfaces are modeled as non-penetrating contact surfaces. The striker bar in this model is given an initial velocity corresponding to that of the test. It is remarked that, at Los Alamos, the striker bar velocity is not routinely measured. The breech chamber pressure for the gun that launches the striker bar is recorded, and a calibration curve is available to determine the striker bar velocity. However, the impact velocity can also be determined from the incident wave strain-time record. The average jump in strain for the incident wave form is related to the impact velocity by equation 2, and this method was the used in this simulation to determine the initial velocity for the striker bar.

$$V_{impact} = \frac{2E\delta\varepsilon}{\rho C_0} \tag{2}$$

Where,

$E =$ Young's Modulus of the Bar Material

$\delta\varepsilon =$ Average Jump in Incident Axial Bar Strain

$\rho =$ Bar Material Density

$C_0 =$ Bar Rod Sound Speed.

This ASCI scale simulation was run on the Los Alamos SGI Blue Mountain computing facility using 64 processors and took about 12 hours to simulate 0.4 ms of the Hopkinson-bar test.

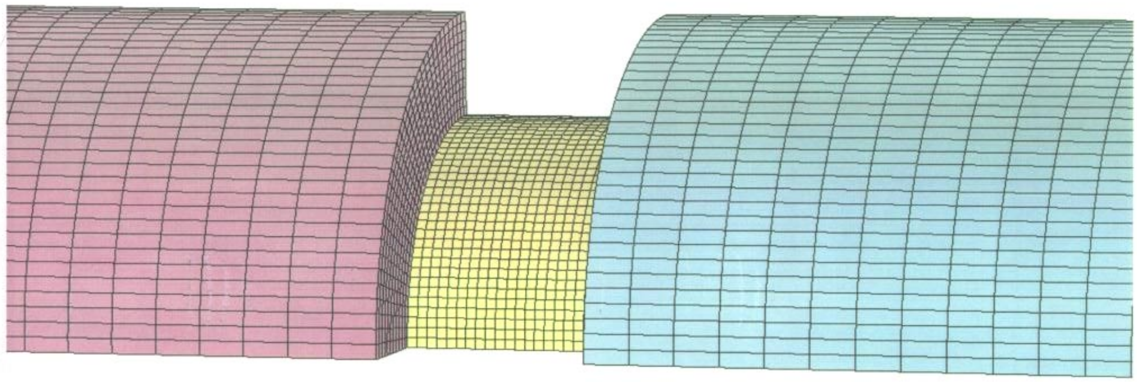

Figure 9 A zoom view on the Hopkinson-bar mesh showing the ViscoSCRAM material specimen as modeled between the incident wave bar and the transmitted wave bar. The faces between the materials are modeled as “contact with sliding friction” interfaces.

The validation methodology used here is to compare the recorded strain gage time histories measured on the incident and transmitted pressure bars with the time history of the simulated strain gages in the FEM. Figure 10 illustrates these strain-time histories, with the upper record being that for the incident bar, and the lower record being that from the transmitted bar record. The titanium bars were modeled with no material damping, but it appears that from the higher frequencies, as evident in the strain gage records, the material does exhibit some damping. The agreement between the experimental record and the simulation is deemed remarkably good, and ViscoSCRAM is seen to capture the high rate response with good fidelity. It is not known at this time whether the difference between the records beginning at about 0.27 ms in the decay history for the transmitted wave can be improved upon with either more Maxwell elements or a slight change in the damage law or is due to experimental scatter. Although the peak dynamic strength has been demonstrated to be relatively constant for PBX 9501 [7], the micro-structural features vary from lot-to-lot which may also affect the global post-peak stress-time response. Thus, the simulation here is deemed excellent in agreement, and adequate to predict the structural response in continuum simulations.

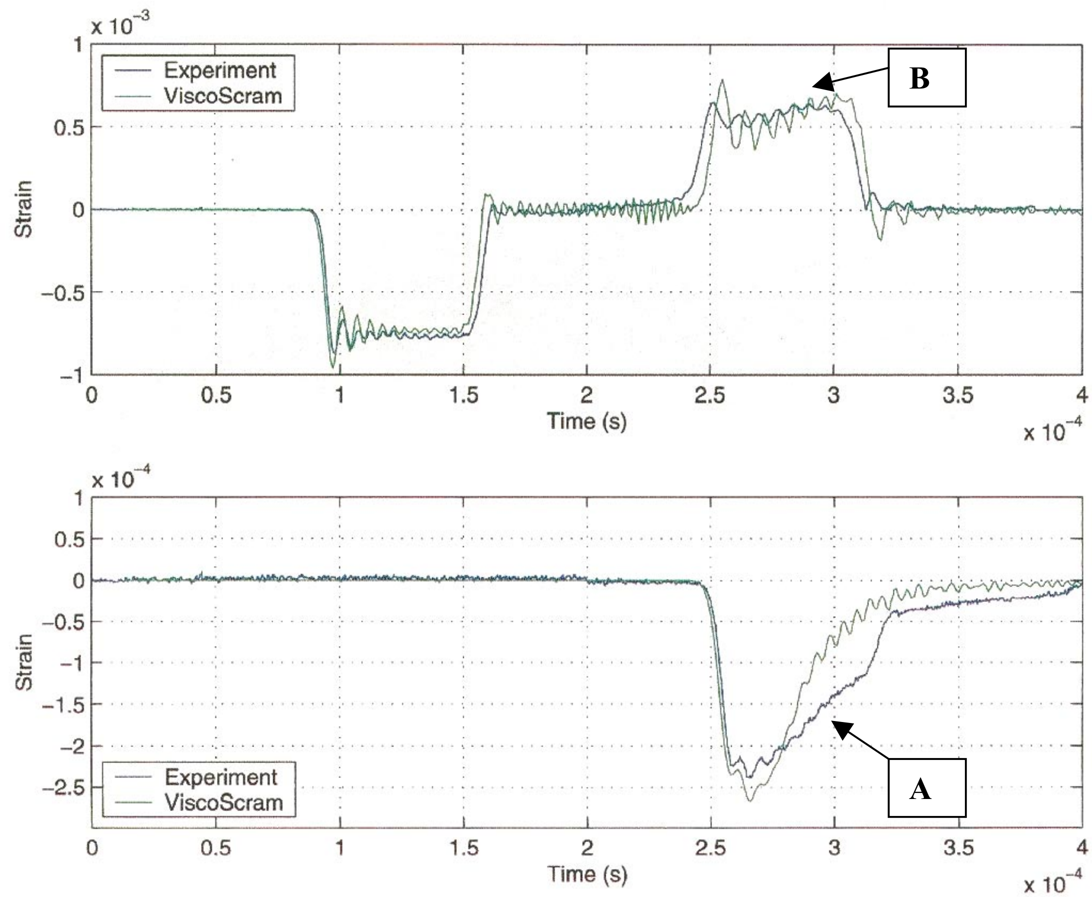

Figure 10 A comparison of the strain-time records from the SHPB records and the simulated strain gages.

The stress vs. time and strain vs. time results are also available from any element in the simulation, and these results may be cross-plotted to obtain the stress vs. strain response in that element for the material. For example, Fig. 11 illustrates such results for a brick element selected from the middle of the modeled sample near the center-line. The cross-plot of stress vs. strain may be compared directly with the SHPB results such as is given in [7], where dynamic data is given for this material as a function of temperature. A portion of the reduced stress-strain data from the actual simulated SHPB test is shown below the cross-plot, and shows that the peak stress after stress state stability was reached was about 58 MPa, with a similar magnitude and result for the cross-plot for the single element result. This comparison is clearly is another method for validation of this complex rate-dependent model.

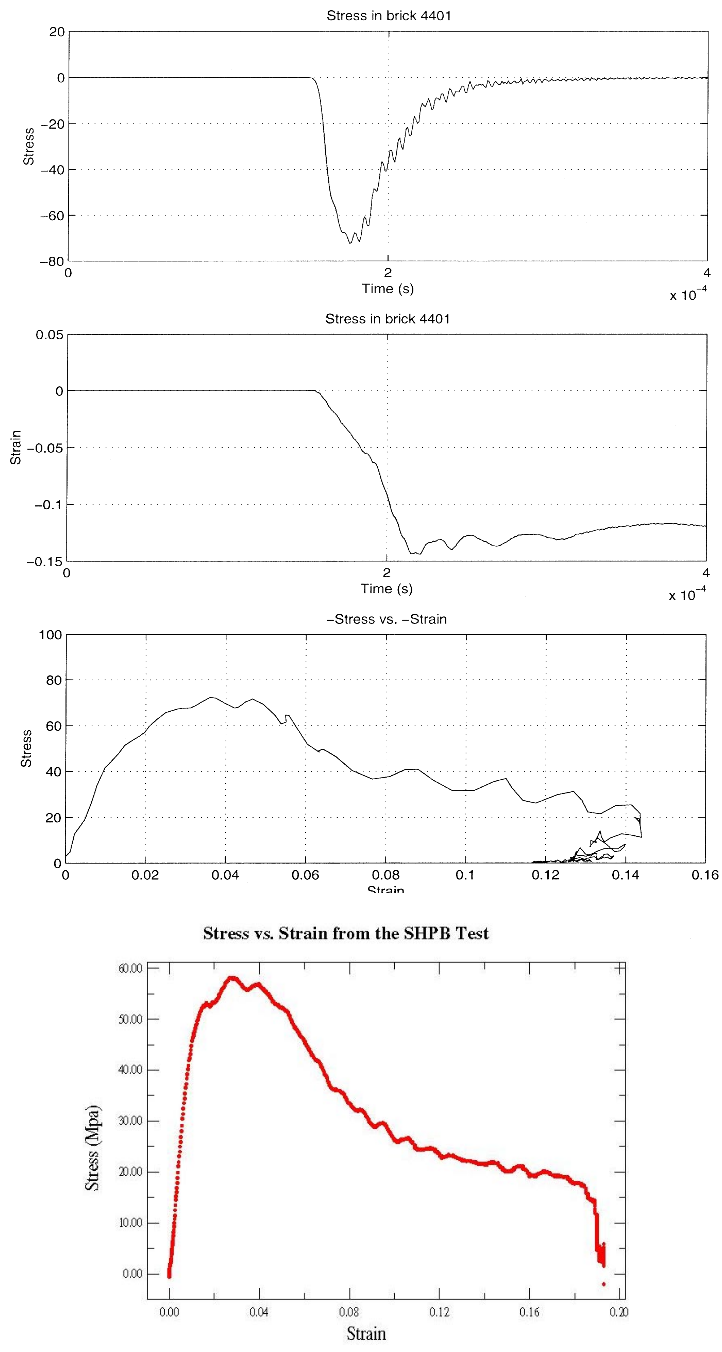

Fig. 11 A plot of the stress-time and strain-time history for a brick element near the center of the modeled SHPB specimen. Below these plots is the resulting cross-plot of stress vs. strain and for comparison, the SHPB reduced data for this simulated test.

Discussion

One point of discussion for the Hopkinson-bar simulation, is that this validation modeling checks more than just the material model's ability to correctly capture the physical response of the material. The chosen FE program's ability to model the contact interface correctly is also tested along with that associated physics. However, the mesh must also be fine enough for the code to simulate the contact interface physics properly. For example, this simulation was first attempted with a FE model that contained ~50,000 elements total, with about 48 elements in the specimen, which gave a 16 specimen element faces in contact with the bars. This mesh, while looking good visually, and *actually did do* an adequate job representing the incident strain-time history, completely *failed* to transmit *any* wave through the specimen, with total reflection at the interfaces producing separation!

Another point of discussion is that the material itself can be variable, with many micro-scale effects that can play a role in the strength. As an example, data has been obtained that indicates as much as a 20% difference in the quasi-static strength of this material at a given strain rate, with a density variation of 1.811 to 1.813 g/cc. ViscoSCRAM is not meant to capture those effects, and although they may influence the behavior locally, the overall structural behavior is captured with the continuum representation as validated here.

The robust nature of the coupling of the constitutive modeling of the PBX 9501 with the damage accumulation input via the ViscoSCRAM model is seen in two ways in the simulation results in Figure 10 compared to the experimental data. First, the rapid decrease in the flow stress of the PBX 9501 after achieving a peak flow stress level is due to the precipitous damage which occurs in the HMX crystals and decohesion between the HMX crystals and the nitroplasticized estane polymer matrix. The comparison between the experimental and simulated transmitted wave signals, denoted by “A” in Figure 10, shows the coupling of the complex constitutive response with the damage accumulation from ViscoSCRAM. The precipitous decrease in the flow stress is due to the rapid evolution of cracking in the PBX 9501. The cracking leads to a reduction in the flow stress, which the sample can sustain. The second indication that the ViscoSCRAM model is capturing the essence of the coupled yield and damage response of the PBX 9501 is seen by examining the strain rate data as a function of time. The strain rate is deduced from the reflected wave signal as denoted by “B” in Figure 10. The strain rate data displays an initial nominally constant strain rate response followed by a ramped increase in the strain rate. This behavior is consistent with cracking damage within the sample, which reduces the ability of the sample to sustain as high a level of stress, and thereafter, upon reduction in the sample length due to the damage and failure processes the effective strain rate increases in the sample. The importance of monitoring the strain rate signal as a function of time in addition to the 1- and 2-wave analysis is shown in this example. While the 1-wave / 2-wave analysis may still suggest a reasonably stable state of stress in the sample, albeit a falling flow stress, the jump in strain rate demonstrates that a non-uniform process, such as cracking, must be on-going. The information presented in Figure 10 indicating the falling flow stress in the transmitted wave and commensurate increase in strain rate when combined support the strong influence of damage on the constitutive response of PBX 9501. Further, this study supports the value of FEM of split-Hopkinson Pressure Bar tests as a means to validate the deformation and failure response of materials subjected to complex loading histories.

Conclusions

The validation methodology for rate-dependent constitutive models illustrated in this paper, uses two different FE technologies that are well developed, the implicit method and the explicit method. Each FE methodology has applications for which one or the other is the best, with the implicit method better suited for modeling quasi-static loading conditions, while the explicit method is better suited for modeling higher rate dynamic loadings. Both methodologies will soon be available for massively parallel applications coming out of the ASCI technology transfer programs from the DOE. Calculations such as the one illustrated in this paper for the Hopkinson-bar simulation will become common-place, Ref(6). The calculations will still be expensive enough in terms of computer/personnel time spent, that validation of the material model by simulation of the higher rate tests for numerous different impact velocities may be impractical. A better strategy may be the one illustrated here, i.e. simulate a single test or a couple of different impact velocity tests and compare directly with the strain-time history records from the data taken on the elastic bars.

Acknowledgements

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